A Maxwellian Path to the q-Nonextensive Velocity Distribution Function

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Abstract

Maxwell's first derivation of the equilibrium distribution function for a dilute gas is generalized in the spirit of the nonextensive q-statistics proposed by Tsallis. As an application, the q-Doppler broadening of spectral lines due to the random thermal motion of the radiating atoms is derived. 05.45.+b; 05.20.-y; 05.90.+m

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It is widely known that the thermodynamical or statistical description of nonextensive systems demand a generalization of the usual Boltzmann-Gibbs thermostatistics [1–3]. A few important examples of physical systems or processes where the standard approach seems to be inadequate are self-gravitating systems, some kinds of plasma turbulence, and self-organized criticality.

The standard Boltzmann-Gibbs approach is based on the extensive entropy measure

$$S = -k \sum_{i} p_i \ln p_i \quad , \tag{1}$$

where k is the Boltzmann constant and $\{p_i\}$ denotes the probabilities of the microscopic configurations. Ten years ago, in order to deal with the above mentioned difficulties associated with nonextensivity, Tsallis [4,5] proposed the following nonextensive form of entropy

$$S_q = k \frac{[1 - \sum_i p_i^q]}{(q - 1)} \quad , \tag{2}$$

where q is a parameter quantifying the degree of nonextensivity. For instance, given a composite system A + B, constituted by two subsystems A and B, which are independent in the sense of factorizability of the microstate probabilities (i.e. $P_{ij}^{(A+B)} = P_i^{(A)} P_j^{(B)}$), the Tsallis measure verifies

$$S_q(A+B) = S_q(A) + S_q(B) + (1-q)S_q(A)S_q(B)$$
(3)

In the limit $q \to 1$, S_q reduces to the standard logarithmic measure (1), and the usual additivity of entropy is recovered. There is a growing body of evidence suggesting that the q-entropy may provide a convenient frame for the thermostatistical analysis of many physical scenarios, such as stellar polytropes [6], turbulence in electronic plasmas [7], anomalous diffusion [8], Levy distributions [9,10], the critical regime in low dimensional dissipative chaotic systems [11–13], the solar neutrino problem [14], peculiar velocity distribution of galaxy clusters [15] or more generally, systems endowed with long range interactions, long range memory effects, or a fractal-like space-time [1,2]. The nonextensive thermostatistics has been shown to be endowed with interesting mathematical properties [16–18], the main theorems of the standard statistics admitting suitable generalizations [19–22]. The issue related

with the connection between q-statistics and q-thermodynamics has also been addressed [5,23], while the time evolution of S_q has been analyzed both in the discrete case through a direct application of the master equation [24], and in the continuous one in connection with the Liouville and Fokker-Planck equations [25]. Some cosmological implications of Tsallis generalized thermostatistics have also been discussed [26,27]. However, at present there is only a limited understanding on the relation between the q parameter and the underlying microscopic dynamics. In the cases of low dimensional dissipative chaotic maps [11,12], and in some toy models of self-organized criticallity [28], the value of q characterizing the system has been obtained from studies of the concomitant dynamics. In spite of the importance of these developments, they do not involve directly the Tsallis maximum entropy distribution and the experimental evidences supporting it. In order to clarify this point, let us briefly review the main observational facts supporting nowadays Tsallis' proposal. First, a Tsallis' maximum entropy distribution has been shown to describe properly a metastable equilibrium state of a 2-dimensional pure electron plasma [7]. Second, the q-distribution corresponding to an ideal classical gas provides a better fit for the observed distribution of peculiar velocities of galaxy clusters than the ones obtained by recourse to more complicated models based on the standard thermostatistics [15]. Finally, assuming a q-velocity distribution for the involved particles, the evaluation of the nuclear reaction rates in the solar interior predicts a neutrino flux in agreement with the observational data, thereby suggesting that Tsallis' thermostatistics may provide a solution for the well-known solar neutrino problem [14].

It is remarkable that all the experimental evidence listed above deals, directly or indirectly, with the q-distribution of velocities, which can be obtained maximizing S_q under the normalization and mean energy constraints. Within a more general framework, such a distribution describes how the q-nonextensive canonical ensemble, associated with the classical many body problem, depends on the particle velocities [29]. In this way, the q-velocity distribution seems to be a reasonable nonextensive generalization of the celebrated Maxwell-Boltzmann distribution, which is recovered as the particular $q \to 1$ limiting case. In spite of its theoretical interest, a satisfactory microscopic explanation for the physical origin of the q-velocity distribution is still lacking, although some interesting attempts have recently been made in connection with the linear and nonlinear Fokker-Planck equations [30]. However, to shed some light on this matters, it seems important to consider suitable (nonextensive) generalizations of the kinetic approach pioneered by Maxwell and Boltzmann.

In this letter, we are interested in exploring the kinetic route. Our aim is to rediscuss the correspondence between the parameter q introduced by Tsallis and the q-equilibrium velocity distribution for a Maxwellian gas, however, assuming from the very beginning a nonextensive generalization of the separability hyphothesis originally proposed by Maxwell [31]. Hopefully, as happened in the extensive framework, this line of inquiry may provide some insight for a more rigorous kinetic irreversible treatment from the Boltzmann viewpoint. As a new application, we deduce a formula for the q-Doppler broadening of spectral lines.

Let us now consider a spatially homogeneous gas, suposed in equilibrium at temperature T, in such a way that $F(\mathbf{v})d^3v$ is the number of particles with velocity in the volume element d^3v around \mathbf{v} . In Maxwell's derivation, the 3-dimensional distribution is factorized (lottery assumption) and depends only on the magnitude of the velocity [31,32]

$$F\left(\sqrt{v_x^2 + v_y^2 + v_z^2}\right)d^3v = f(v_x)f(v_y)f(v_z)dv_xdv_ydv_z \quad , \tag{4}$$

from which it is straightforward to show that

$$f(v_i) = A_1 e^{-\frac{\beta m v_i^2}{2}}$$
 , $i = x, y, z$ (5)

and

$$F(\mathbf{v}) = A_1^3 e^{-\frac{\beta m v^2}{2}} \quad , \tag{6}$$

where $\beta = \frac{1}{kT}$ in order to recover the standard macroscopic thermodynamic relations, and $A_1 = \sqrt{\frac{m}{2\pi kT}}$ is the normalization constant. Naturally, in the nonextensive context described by (2), the starting basic hypothesis (4), which takes into account the isotropy of all velocity directions, must somewhat be modified. Physically, Maxwell's ansatz is tantamount to assume that the three components of the velocity are uncorrelated. However, this property

does not hold in the systems endowed with long range interactions where Tsallis distribution has been observed [7,14,15]. Notice that the Maxwell ansatz is equivalent to express $\ln F$ as the sum of the logarithms of the one dimensional distribution functions associated with each velocity component. A simple and natural way to generalize this procedure within the nonextensive formalism, in order to introduce correlations between the velocity components, would be to replace the logarithm function by a power law. However, in order to recover the ordinary logarithmic ansatz as a particular limiting case, it is convenient to express the power generalization in terms of the q-log function, which is a combination of a power function plus appropriate constants. Elementary considerations may convince oneself that a consistent q-generalization of (4) is (for simplicity we provisionally consider the bidimensional case)

$$F\left(\sqrt{v_x^2 + v_y^2}\right) d^2v = e_q(f^{q-1}(v_x) \ln_q f(v_x) + f^{q-1}(v_y) \ln_q f(v_y)) dv_x dv_y \quad , \tag{7}$$

where the q-exp and q-log functions, $e_q(f)$, $\ln_q(f)$, are defined by

$$e_q(f) = [1 + (1-q)f]^{1/1-q}$$
 , (8)

$$\ln_q f = \frac{f^{1-q} - 1}{1 - q} \quad . \tag{9}$$

As one may check, $e_q(\ln_q f) = \ln_q(e_q(f)) = f$, and from (9) we see that the q-log differentiation, $\frac{d}{dx} \ln_q f = f^{-q} \frac{df}{dx}$ is also satisfied. Note also that in the limit $q \to 1$ the identities (8)-(9) reproduce the usual properties of the exponential and logarithm functions, and (7) reduces to the bidimensional case of (4), as should be expected. Now, partial q-log differentiation of (7) with respect to v_x yields

$$\frac{\partial \ln_q F}{\partial v_x} = \frac{\partial \ln_q \left[e_q(f^{q-1}(v_x) \ln_q f(v_x) + f^{q-1}(v_y) \ln_q f(v_y)) \right]}{\partial v_x} \quad , \tag{10}$$

or equivalently,

$$\frac{v_x}{\chi} \frac{F'(\chi)}{F^q(\chi)} = \frac{\partial}{\partial v_x} \{ f^{q-1}(v_x) \ln_q f(v_x) \} \quad , \tag{11}$$

where $\chi = \sqrt{v_x^2 + v_y^2}$ and a prime means total derivative. Note that analogous equations apply to the remaining components even whether we had considered the n-dimensional case. Introducing the shorthand notation

$$\Phi(\chi) = \frac{1}{\chi} \frac{F'(\chi)}{F^q(\chi)} \quad , \tag{12}$$

we may rewrite (11) as

$$\Phi(\chi) = \frac{1}{v_x} \frac{\partial}{\partial v_x} \{ f^{q-1}(v_x) \ln_q f(v_x) \} = \frac{1}{v_y} \frac{\partial}{\partial v_y} \{ f^{q-1}(v_y) \ln_q f(v_y) \}.$$
(13)

The second member of the above equation only depends on v_x , while the third one is a function exclusively of variable v_y . Hence, equation (13) can be satisfied only if all its members are equal to one and the same constant, not depending on any of the velocity components. So, we may put $\Phi(\chi) = -m\gamma$, where m is the mass of the particles and γ is an arbitrary constant. Of course, the introduction of m at this point is dictated only by the known Maxwellian limit. As one may see from (9), $f^{q-1}(v_x) \ln_q f(v_x) = \ln_{q^*} f(v_x)$, where $q^* = 2 - q$. Hence, the general solutions for $f(v_x)$ is given by (equivalent expressions are valid for $f(v_y)$ and $f(v_z)$)

$$\ln_{q^*} f(v_x) = -\frac{m\gamma}{2} v_x^2 + \ln_{q^*} A \quad , \tag{14}$$

where, without loss of generality, we have written the integration constant in a convenient form. Now, taking the q-exponential in both sides of (14) it follows that

$$f(v_x) = \left[1 + (1 - q^*) \left(\ln_{q^*} A - \frac{\gamma m v_x^2}{2} \right) \right]^{1/1 - q^*} , \qquad (15)$$

and defining a new constant β as

$$\beta = \frac{\gamma}{1 + (1 - q^*) \ln_{q^*} A} = \frac{\gamma}{A^{1 - q^*}} \quad , \tag{16}$$

we find the generalized expression

$$f(v_x) = A_q \left[1 - (q-1) \frac{\beta m v_x^2}{2} \right]^{\frac{1}{q-1}} , \qquad (17)$$

where we have introduced a subindex q to make explicit the q-dependence of A. From (17) we see that the Gaussian probability curve of the Maxwellian gas is replaced by the charactheristic power law behavior of Tsallis' nonextensive framework, and as expected, the limit q=1 recovers the exponential extensive result. Note also that for values of q greater than unity, the positiviness of power argument means that (17) exhibits a thermal cut-off in the maximal allowed velocities. The components of the velocities lie on the interval [-L, L], where $L=\sqrt{\frac{2}{m\beta(q-1)}}$. Hence, the integration limits in the standard normalization condition is modified in such a way that only if q=1 they go to infinity. Taking this into account one may show that the normalization constant A_q can be expressed in terms of Gamma-functions as

$$A_{q} = \left(\frac{1+q}{2}\right) \frac{\Gamma(\frac{1}{2} + \frac{1}{q-1})}{\Gamma(\frac{1}{q-1})} \sqrt{\frac{m(q-1)}{2\pi kT}} \quad . \tag{18}$$

Further, using that $\lim_{|z|\to\infty} \frac{\Gamma(a+z)}{\Gamma(z)} e^{-a \ln z} = 1$ (see Abramowitz [33]), it is easy to see that A_1 is the standard Maxwellian result.

Before continuing we need to obtain the complete distribution. By adding the v_z component to (7) it is readily seen that

$$F\left(\sqrt{v_x^2 + v_y^2 + v_z^2}\right) d^2v = e_q(\ln_{q^*} f(v_x) + \ln_{q^*} f(v_y) + \ln_{q^*} f(v_z)) dv_x dv_y dv_z \quad . \tag{19}$$

Hence, taking the q-logarithim of the above expression and repeating the same algebraic steps of the one-dimensional case it follows that

$$F(\mathbf{v}) = B_q \left[1 - (q-1) \frac{\beta m v^2}{2} \right]^{\frac{1}{q-1}} ,$$
 (20)

where B_q is fixed by the 3-dimensional normalization condition. We find

$$B_q = (q-1)^{1/2} \frac{(3q-1)}{2} \left(\frac{1+q}{2}\right) \frac{\Gamma(\frac{1}{2} + \frac{1}{q-1})}{\Gamma(\frac{1}{q-1})} \left[\frac{m}{2\pi kT}\right]^{\frac{3}{2}} . \tag{21}$$

As expected, the q-distribution (20) is isotropic meaning that all velocity directions are also equivalent in this generalized context. As remarked earlier for the one-dimensional case, there also exist a temperature dependent cut-off on the magnitude of the velocities. From

(18) we see that the $B_1 = A_1^3 = \left[\frac{m}{2\pi kT}\right]^{\frac{3}{2}}$ is the standard 3-dimensional Maxwellian result as it should be.

Now we discuss an important point of principle, which is related with the definition of marginal probabilities in the context of q-statistics. In ordinary space, a marginal probability, say, $f(v_x)$, may be obtained from the 3-dimensional distribution by

$$f(v_x) = \int F(v_x, v_y, v_z) dv_y dv_z \quad . \tag{22}$$

This elementary and natural definition, widely applied in statistical physics, is not usually regarded as deserving any further scrutiny. However, within the nonextensive framework we are discussing here, the concept of marginal probability distributions shows some new remarkable features. Basically, this occurs because the distribution $f(v_x)$, as given by (22), does not coincid with our equation (17). As one may check, it has a power different from $\frac{1}{q-1}$. In other words, using the above formula, the 3-dimensional distribution (20) leads to a $f(v_x)$ with a different value of q. Strictly speaking, since the q-distribution cannot be factorized, the power of the one-dimensional distribution obtained from a marginal probability like (22), depends on the number of spatial dimensions. The power increases by $\frac{1}{2}$ for each additional dimension present in the complete distribution. This is equivalent to say that $f(v_x)$ is also a power law, but with an effective q-parameter. However, to interpret this fact in a consistent way, it is required to introduce an effective temperature in the one-dimensional distribution. Naturally, the same happens when we consider arbitrary dimensions m, n, where m < n. In particular, this means that the zeroth law of thermodynamics is not satisfied for systems described in this nonextensive framework. Hopefully, a proper modification of (22) can be found which avoids these undesirable features, but preserves the interesting ones. In this concern, we suggest the following general expression for the marginal m-dimensional distribution in a n-dimensional q-velocity space

$$f(v_1, v_2, ..., v_m) = \frac{\int F^{\alpha}(v_1, v_2, ..., v_n) dv_{m+1} dv_{m+2} ... dv_n}{\int F^{\alpha}(v_1, v_2, ..., v_n) dv_1 dv_2 ... dv_n} ,$$
 (23)

where $\alpha = 1 - \frac{1}{2}(q-1)(n-m)$. For q=1, we have $\alpha = 1$, and the standard definition is recovered. In the above discussed case, n=3, m=1, one finds $\alpha = 2-q$. For this value

of α it is straightforward to show that (23) reproduces the one-dimensional distribution (17). As a matter of fact, our prescription (23) solves the conflict with the zeroth law of thermodynamics, in the sense that the same power law and temperature of the complete distribution is always obtained regardless of the specific dimensions involved in the problem. Besides, it is interesting to realize that equation (23) can be interpreted as defining the ordinary marginal probability function computed using the escort distribution [34]

$$F^* = \frac{F^{\alpha}}{\int F^{\alpha} d^N v},\tag{24}$$

instead of being evaluated using the original distribution F. This is a standard procedure in the fractal thermodynamic formalism [34].

Broadening of Spectral Lines. The random motion of particles broadens spectral lines, first, because of collisions between the particles (pressure broadening), and second, due to the thermal Doppler effect of the radiating atoms. As widely known, in the extensive case the first effect is proportional to $pT^{-\frac{1}{2}}$, where p is the pressure, whereas the second scales with $T^{\frac{1}{2}}$. Let us now discuss the latter effect using the q-Maxwellian velocity distribution. The standard result was derived by Lord Rayleigh and further observed by Michelson [35,36].

In order to estimate the magnitude of the q-Doppler broadening for the visible light emitted by the molecules of a hot gas, it is enough to consider the one dimensional case. Neglecting relativistic effects, the frequency shift viewed along the x direction is given by the standard Newtonian formula

$$\nu = \nu_0 \left(1 + \frac{v_x}{c} \right) \quad . \tag{25}$$

The frequency distribution expected for a spectral line centered at ν_0 is obtained changing variables from v_x to ν . From (17) it is readily seen that

$$f(\nu)d\nu = A_q \left[1 - (q-1)\frac{mc^2}{2kT} \left(\frac{\nu - \nu_o}{\nu_o}\right)^2 \right]^{\frac{1}{q-1}} \frac{c}{\nu_o} d\nu \quad , \tag{26}$$

which has also the form of a Maxwellian q-distribution. The broadening is usually measured by the width of the spectral line at half intensity. It is easy to check that in terms of the wavelenght, the standard deviation is replaced by

$$\Delta \lambda_d = \lambda_o \left[\frac{2kT}{mc^2} \left(\frac{1 - 2^{1-q}}{q - 1} \right) \right]^{1/2} = \lambda_o \left(\frac{kT}{mc^2} 2 \ln_q 2 \right)^{1/2} . \tag{27}$$

For q=1 the standard result is recovered as should be expected [32,35]. However, although mantaining the same $T^{\frac{1}{2}}$ temperature dependence, the thermal Doppler broadening is modified in the nonextensive framework. Naturally, the above formula can be used to limit the q-parameter. Note that in a log-log plot of $\Delta \lambda_d$ versus $\frac{kT}{mc^2}$, the straight line is displaced parallel to itself for each value of q different from unity. In comparison with the standard q=1 result, the above q-velocity distribution gives a narrowing of the Doppler width for q<1, and a broadening tendency for q larger than unity.

Tsallis' Generalized Mean Values. It is worth noticing that we might have considered a different generalization for the factorization condition. In principle, instead of equation (7) one may assume the following ansatz

$$F = e_q(\ln_q f(v_x) + \ln_q f(v_y)).$$
 (28)

In this case, repeating the same steps we have already explained, instead of (17), one obtains a slightly different velocity distribution

$$f(v_x) = A_q \left[1 - (1 - q) \frac{1}{2} \beta m v_x^2 \right]^{\frac{1}{1 - q}}, \tag{29}$$

which is exactly that one determined by Tsallis MaxEnt prescription when the generalized mean value [5]

$$\langle v_x^2 \rangle_q = \int f^q \, v_x^2 \, dv_x \tag{30}$$

is a meaningful constraint. On the other hand, by employing the standard linear mean values, distribution (17) is obtained. As a matter of fact, none of the main results and conclusions of this paper change in a significative way whether one adopts the alternative factorization prescription (28). For instance, all the results corresponding to our analysis of the q-Doppler broadening follow simply by replacing everywhere (q-1) by (1-q). This is a strong indication that a more conclusive result needs a full kinetic theoretic treatment, which requires a proper generalization of the Boltzmann H-theorem.

It is possible that the approach developed here may be implemented even if more general expressions for nonextensive entropies, which reduce in a common limit to the Boltzmann-Gibbs-Shanon form, are considered. Tsallis measure S_q is not the only conceivable mathematical generalization of the standard logarithmic entropy. Other interesting nonextensive entropic functionals have been recently proposed [37,38]. However, Tsallis entropy has been shown to be endowed with many elegant and useful mathematical properties, and its associated q-MaxEnt distributions have been experimentally observed [7,15]. It would be of great interest to explore the, so far poorly known, mathematical properties of the recently introduced entropies [37,38], as well as to determine if they admit relevant physical applications. Conclusions. In the present work we have obtained Tsallis non-extensive velocity distribution by recourse to an argument akin to the celebrated derivation advanced by Maxwell for the equilibrium velocity distribution. As shown by Maxwell, his distribution is the only one compatible with isotropy and factorizability with respect to each velocity component. Similarly, Tsallis q-distribution is uniquely determined by the requirements of (i) isotropy, and (ii) a suitable generalization of the factorizability condition. Maxwell's factorization condition is tantamount in requiring that the *logarithm* of the complete distribution function be equal to a sum of N terms, each one depending only on one velocity component. Instead of logarithm, our factorization condition requires that a power of the complete distribution be equal to a sum of N terms, which also depend only on one velocity component. Reformulating this last condition in terms of the Tsallis q-logarithm function, Maxwell's expressions are recovered in the $q \to 1$ limit. The same happens with the formula giving the broadening of spectral lines.

It is important to stress that the simple transformation $(q-1) \to (1-q)$ is enough to recast all the present results within the complete Tsallis formalism [5] based on Tsallis generalized mean values. In that case, Tsallis q-distribution would adopt the form

$$F(\mathbf{v}) = \tilde{B}_q \left[1 - (1 - q) \frac{\beta m v^2}{2} \right]^{\frac{1}{1 - q}} , \qquad (31)$$

where \tilde{B}_q is given by the expression obtained from (21) after replacing (q-1) by (1-q).

In a similar vein, the q-Doppler width of spectral lines would appear under the guise

$$\Delta \lambda_d = \lambda_o \left(\frac{kT}{mc^2} 2^q \ln_q 2 \right)^{1/2} . \tag{32}$$

Mathematically, Maxwell factorization condition is similar to the Maxwell-Boltzmann hypothesis of "molecular chaos", which assumes that the two-molecule distribution function describing the colliding molecules is factorizable as the product of two one-molecule distributions (i.e. $F(\mathbf{v}_1, \mathbf{v}_2) = f(\mathbf{v}_1) f(\mathbf{v}_2)$). This hypothesis plays a fundamental role in the standard kinetic theory of gases [32]. Boltzmann' proof that any initial velocity distribution evolves irreversibly towards Maxwell's distribution does not rely just in the general principles of classical mechanics. It also needs the additional assumption of "molecular chaos". Boltzmann himself [39] recognized that the hypothesis of "molecular chaos" may not always hold, especially at high densities. Our present results suggest that Boltzmann's approach to Maxwell's velocity distribution can be adapted to the non-extensive setting by recourse to an appropriate generalization of the "molecular chaos" assumption. This issue will be addressed in a forthcoming communication.

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